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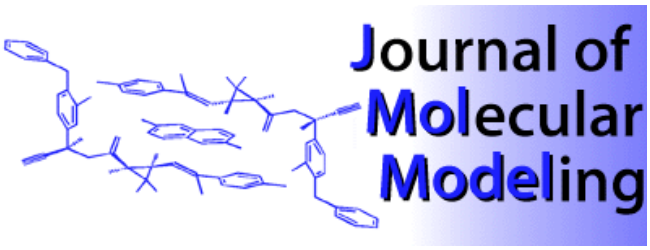

Book Review

Encyclopedia of Computational Chemistry

Schleyer, P.v.R; Allinger, N.L.; Clark, T.; Gasteiger, J.; Kollman, P.A.; Schaefer III, H.F.; Schreiner, P.R., Eds.; John Wiley & Sons: Chichester, UK, 1998; Volume 1-5. ISBN 0-471-96588-X. £ 1950.– / $ 3150.– / EUR 3017.14 (recommended price)

If you need a good entry point to a given topic, you can of course expect to find it somewhere in the Internet, but how do you find it? Traditionally, people prefer a library, or even better, their own bookshelf. The ideal situation is to have all the information on a topic or area of interest available (up to a certain time, of course) in a series of books, hopefully equipped with a detailed index. This leads us to an encyclopedia on that area, in this case computational chemistry.

The idea to concentrate the current knowledge on a given subject in a series of articles is not new. Well known examples are the "Topics in Current Chemistry" or the "Reviews of Computational Chemistry", to name only two. However, these types of publications grow continuously, without the reader knowing the focus of the next volume. The Encyclopedia of Computational Chemistry (ECC) goes a different way. Representing a state-of-the-art collection of information on almost all topics a computational chemist might interest, ECC should ideally be a complete compilation of the necessary information. This is in fact largely true.

Conceptually, there are three types of entries in the ECC: (1) *regular articles*: composed by a specialist on the field, they all have essentially the same general structure – abbreviations, glossary of terms, main text, related articles, references – and give in a few pages a sophisticated introduction into the topic. It should also be noted that these review-like contributions are fully citable. (2) *definition entries*: explaining certain terms commonly used in computational chemistry in short, they follow the official IUPAC recommendations. (3) *descriptions of software packages*: the last volume of the ECC holds an extra section for some commercial software descriptions provided by the companies involved.

Now let us look at some technical details. The ECC comes in five hard-covered volumes with a total of about 3500 double columned pages. Besides preface and synopses each volume contains the complete table of contents, which is separated according to the volume contents; a list of often used abbreviations is included on the endpapers. Beyond that, the last volume provides a detailed subject index and a list of contributors.

Some additional statistics for the interested: regular articles (ca. 320) and definition entries (ca. 360) occupy 3266 pages, and 25 software packages are described on 80 pages. The list of contributors contains 24 pages and the detailed index 44 pages. Over 1400 illustrations, 280 full color, enhance the presentation.

Clearly, the nature of an encyclopedia is not suitable for a summary in the common sense. However, to provide an overview, we will give in the following the section editors' synopses in brief.

Peter Kollman is responsible for the section "Computational chemistry applied to systems of biological interest", that covers force fields for molecular mechanics and dynamics, methods and applications for macromelocular simulations, application of molecular simulation methods to biochemical systems, structural refinement and analysis, solvent continuum models, conformational analysis, ligand and drug design, QM/MM-methods, macromolecular properities and their modeling.

The field of cheminformatics ("Computational chemistry beyond calculations") was supervised by Johann Gasteiger. The main topics therein are structure representation and manipulation (generation, visualisation, and nomenclature), structure analysis and searching (numbering, 3D search, graph theory), databases (literature, structures, reactions, data), information access (Internet, electronic publishing, online services), data analysis methods (artificial intelligence, genetic algorithms, fuzzy logic, neural networks, object-orientated programming, partial least squares), data analysis process (data processing, reactions information, structure/spectra correlations), knowledge based systems (biodegradation, chemical engineering, synthesis design) and drug design (combinatorial chemistry, protein structure prediction in 1D, 2D, 3D, QSAR, *de novo* design).

Paul von Ragué Schleyer – this name is probably one of the first associated with the application of quantum chemical calculations. Therefore, the reader will not be surprised that Schleyer not only acted as editor-in-chief, but also as section editor for "Numerical computational chemistry for the general user". The main focus here is on programs that

both specialists in theoretical chemistry and nonspecialists like practial working chemists can use with success.

The general section about "Molecular mechanics" is Lou Allinger's. Almost all aspects of force fields (general analytic form, parametrisation, molecular dynamics, Monte Carlo simulations etc.), their advantages as well as their disadvantages are treated. Detailed attention is given to some popular force field implementations (CHARMM, CFF, MM1-3, MMFF, GROMOS).

"More purely theoretical aspects of computational chemistry" is the title of Henry Schaefer III's section. It deals with theory and application of *ab initio* methods, density functional theory, molecular properties other than energy, general interpretation of wavefunctions and QM calculation results, QM prediction of large molecular systems, non-covalent bonded systems, theory of dynamics, statistical mechanics for condensed phases and cluster, surface and solid chemistry.

Finally, the "Semiempirical molecular orbital theory" section is taken care of by Tim Clark. Common methods (AM1, MNDO, MNDO/d, PM3, SAM1, PRDDO, INDO, SINDO, configuration interaction, population analysis, COSMO) are described as well as more recent developments like the use of Green's functions in semiempirical MO theory.

This overview of the synopses shows the vast spectrum of topics covered by the ECC. Thus, the reader is very likely to find what he is looking for, presumable even more.

There are only some minor shortcomings in the ECC, e.g. the index searched for the keyword *force field* does not list all force fields treated and an entry about the *universal force field* (UFF) is totally missing, the definition entries are partly very condensed, and the software description seems a bit selective (e.g. GAMESS is not mentioned). Other than this, an optional CD-ROM version of the ECC for advanced searching utilising hyperlinks would have been a helpful addition. An electronic version of the ECC – announced in the software descriptions preface – will have an updated software list.

Taken in all in all, the ECC provides both a quick introduction into various topics of modern computational chemistry through short definition entries and uniformly organised regular articles, and a valuable source for further reading through elaborated reference sections. Numerous illustrations paired with a appealing layout tempt the reader to follow the links to related articles and to read on just for curiosity. Thus, the ECC is suitable for occasional users as well as for specialists who need detailed information about computational techniques. In our eyes the ECC is a must for every group, department or company library, as it serves both computational and experimental chemists.

Supplementary material available statement A detailed list of all contributors in pdf format, made available by the publisher, accompanies this review.

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